

Another method to solve Dirac's one-electron equation numerically

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Abstract. One more mode developed to get eigen energies and states for the one-electron Dirac's equation with spherically symmetric bound potential. For the particular case of the Coulomb potential it was shown that the method is free of so called spurious states. The procedure could be adapted to receive highly excited states with great precision.

1. Introduction

It's difficult to overestimate the importance for the relativistic calculations numerical approaches to get full spectra of Dirac's equation. One of the most successful is so called B-spline approach (Carl de Boor 1978), (Johnson et al. 1988). While numerical implementation of the problem so called spurious states can arise. Those states need special treatment (Shabaev et al. 2004). All said above prompts to explore new methods to solve Dirac's equation numerically. Namely in this paper we'll investigate the advantages that squared Hamiltonian is able to give for reaching the goal. Throughout in the paper atomic units system ($\hbar = e = m$) is utilized.

2. Squared Dirac's Hamiltonian

Let's take the squared one-electron Dirac's Hamiltonian in the form:

$$H = (h - \epsilon)^2 \quad (1)$$

Where $h = c(\alpha \cdot p) + V + mc^2\beta$ is a well-known representation of the one-electron Dirac's Hamiltonian (Labzowsky et al. 1993) with some bound potential V and ϵ is an arbitrary real-valued parameter. Having deployed the (1) everybody can easily receive

$$\begin{aligned} H = & c^2(\alpha \cdot p)^2 + m^2c^4 + V^2 + mc^3\{(\alpha \cdot p), \beta\} + c\{(\alpha \cdot p), V\} + \\ & 2mc^2\beta V - 2\epsilon h + \epsilon^2 \end{aligned} \quad (2)$$

where $\{a, b\} = ab + ba$ is a positive commutator of the operators a and b . Keeping in mind that the fourth term in the above formulae (2) amounts to zero (due to the properties of the Dirac's matrixes) one can finally get

$$H = -\hbar^2 c^2 \Delta + m^2 c^4 + V^2 + 2mc^2 \beta V - i\hbar c \{(\alpha \cdot \nabla), V\} + 2ic\hbar\epsilon(\alpha \cdot \nabla) - 2\varepsilon V - 2\varepsilon mc^2 \beta + \epsilon^2 \quad (3)$$

where for the Coulomb potential $V = -\frac{e^2 Z}{r}$, e and Z are an electron charge and charge number of the nucleus respectively. Our further purpose is to solve the eigen problem for the squared Dirac's equation

$$H\Psi = \lambda\Psi \quad (4)$$

numerically. It's clear that $\lambda = (E - \epsilon)^2$ where E is an eigen number for the h operator. In order to reach that goal one can adapt the usual representation for the eigen function of the Dirac's equation with spherically symmetric bound potential (Labzowsky et al. 1993). Namely let's take

$$\Psi = \begin{pmatrix} g\Omega_{jlm} \\ if\Omega_{j\bar{l}m} \end{pmatrix} \quad (5)$$

that is well-known representation for the Dirac's bispinor, $g = g(r)$ and $f = f(r)$ are upper and lower radial component functions respectively. For the purpose of numerical implementation one needs to expand those functions over finite set of basis functions. We used here finite basis constructed from the B-splines (see for example (Johnson et al. 1988)). So if one has got the finite basis set $\{B_i(x)\}_{i=1}^n$ it's straight forward to gain the generalized symmetric eigen value matrix problem for the equation (4)

$$\begin{pmatrix} H^{(1)} & H^{(2)} \\ H^{(3)} & H^{(4)} \end{pmatrix} x = \lambda \begin{pmatrix} B^{(1)} & 0 \\ 0 & B^{(2)} \end{pmatrix} x \quad (6)$$

Where $H^{(1)}$, $H^{(2)}$, $H^{(3)}$, $H^{(4)}$, $B^{(1)}$, $B^{(2)}$ are the sub-matrixes ($n \times n$) of the general matrixes H and B ($2n \times 2n$), with the matrix elements

$$B_{ij}^{(1)} = B_{ij}^{(2)} = (B_i r^2 B_j) \quad (7)$$

$$\begin{aligned} H_{ij}^{(1)} = & -\hbar^2 c^2 ((B_i r^2 B_j'') + 2(B_i r B_j') - l(l+1)(B_i B_j)) + \\ & m^2 c^4 (B_i r^2 B_j) + (B_i r^2 V^2 B_j) + 2mc^2 (B_i r^2 V B_j) - \\ & 2\epsilon mc^2 (B_i r^2 B_j) - 2\epsilon (B_i r^2 V B_j) + \epsilon^2 (B_i r^2 B_j) \end{aligned} \quad (8)$$

$$\begin{aligned} H_{ij}^{(2)} = & -c\hbar (2(B_i r^2 V B_j') + 2(1-\kappa)(B_i r V B_j) + (B_i r^2 V' B_j)) + \\ & 2\epsilon c\hbar ((B_i r^2 B_j') + (1-\kappa)(B_i r B_j)) \end{aligned} \quad (9)$$

$$\begin{aligned} H_{ij}^{(3)} = & c\hbar (2(B_i r^2 V B_j') + 2(1+\kappa)(B_i r V B_j) + (B_i r^2 V' B_j)) - \\ & 2\epsilon c\hbar ((B_i r^2 B_j') + (1+\kappa)(B_i r B_j)) \end{aligned} \quad (10)$$

$$\begin{aligned} H_{ij}^{(4)} = & -\hbar^2 c^2 ((B_i r^2 B_j'') + 2(B_i r B_j') - \bar{l}(\bar{l}+1)(B_i B_j)) + \\ & m^2 c^4 (B_i r^2 B_j) + (B_i r^2 V^2 B_j) - 2mc^2 (B_i r^2 V B_j) + \\ & 2\epsilon mc^2 (B_i r^2 B_j) - 2\epsilon (B_i r^2 V B_j) + \epsilon^2 (B_i r^2 B_j) \end{aligned} \quad (11)$$

besides $(f) = \int_0^\infty f(r) dr$.

3. Spectra quality test, $\epsilon = 0$ operator

To examine the grade of the spectra Bi H-like ion was chosen. The knot net sequence for the B-spline construction was taken in accordance with the formula $k(i) = \frac{(b-a)}{n^6}i^6 + a$. The boundary conditions were adapted and $f(a) = f(b) = g(a) = g(b) = 0$ in order to prevent the kinetic energy not to be negative. The outcome of the calculation (diagonalization of (4) with $\epsilon = 0$) is presented in Table 1. In Table 1 the lowest eigen values are compared not only with the corresponding eigen values gained from Sommerfeld formula but also with the eigen values received from the virial relations (12, 13). The virial theorem for the operator h and h^2 yields formulae

$$E = mc^2 \langle \Psi | \beta | \Psi \rangle \quad (12)$$

and

$$E^2 = m^2 c^4 + mc^2 \langle \Psi | V\beta | \Psi \rangle \quad (13)$$

respectively. As one can see from Table 1 the agreement is quite good. In addition to this different spectra (especially with $\kappa > 0$) were analyzed and it was found out the absence of so called spurious states. To avoid problems with spurious states special care needs while numerical implementation of the equation $h\Psi = E\Psi$ (Shabaev et al. 2004).

Table 1. Several lowest energy levels for Bi H-like ion with $l = 0$, $j = \frac{1}{2}$. The order of splines $k = 6$ and the number of intervals for the B-splines construction is $n = 130$. Parameters for the knot sequence construction are $a = 10^{-15}$ and $b = 10$ respectively. E stands for self energy value gained by diagonalization of the equation (4). E_S means values received from Sommerfeld's formula. The virial theorem tests are also presented. The E_{vr1} and E_{vr2} columns give the self energies received with formulae (12) and (13) respectively.

E_S	E	E_{vr1}	E_{vr2}
-3836.36956	-3836.36901	-3836.36498	-3836.36583
-984.921152	-984.921036	-984.920525	-984.920581
-425.768940	-425.768909	-425.768766	-425.768777
-234.607639	-234.607627	-234.607570	-234.607573
-148.000373	-148.000368	-148.000340	-148.000340
-101.712322	-101.712319	-101.712304	-101.712304
-74.1444640	-74.1444625	-74.1444530	-74.1444528
-56.4227560	-56.4227552	-56.4227489	-56.4227487
-44.3652984	-44.3652978	-44.3652936	-44.3652933
-35.7940987	-35.7940983	-35.7940953	-35.7940951
-29.4849330	-29.4849328	-29.4849305	-29.4849304

4. The states from continuous part of spectra

As one can see the outcome of the diagonalization of the equation (4) with $\epsilon = 0$ yields for the eigen values corresponding to the continuous part of spectra to be doubly degenerated. In general case the wave function Ψ (for that part of spectra) is a mix of the couple of functions φ_+ (really the self energy function of the h operator with the corresponding self energy $E > 0$) and φ_- (really the self energy function of the h operator with the corresponding self energy $-E$)

$$\Psi = C_1\varphi_+ + C_2\varphi_- \quad (14)$$

with some arbitrary coefficients C_1 and C_2 . Utilizing the properties of the self energy functions (15), (16) and (17)

$$h\varphi_+ = E\varphi_+ \quad (15)$$

$$h\varphi_- = -E\varphi_- \quad (16)$$

$$h\Psi = C_1E\varphi_+ - C_2E\varphi_- \quad (17)$$

one can easily separate the positive and negative spectra functions.

$$h\Psi + E\Psi = 2C_1E\varphi_+ \quad (18)$$

$$h\Psi - E\Psi = -2C_2E\varphi_- \quad (19)$$

Finally the formulae (18) and (19) present the desired functions. Everyone can also easily see that those functions are orthogonal (They really must be!). The formula (20) gives the proof of the fact.

$$\begin{aligned} \langle \varphi_+ | \varphi_- \rangle &= -(4C_1C_2E^2)^{-1} \langle h\Psi + E\Psi | h\Psi - E\Psi \rangle = \\ &= -(4C_1C_2E^2)^{-1} \langle \Psi | (h+E)(h-E) | \Psi \rangle = \\ &= -(4C_1C_2E^2)^{-1} \langle \Psi | h^2 - E^2 | \Psi \rangle = 0 \end{aligned} \quad (20)$$

To conclude this section we can say that there is no problem to get full spectra and eigen functions of Dirac's one-electron Hamiltonian from the squared one.

5. The $\epsilon \neq 0$ operator

The case of the operator (4) with $\epsilon \neq 0$ is very interesting one. When $\epsilon = 0$ the spectra of the operator (4) looks like one of the Schrodinger equation, namely we have two part spectra, the lowest energies are bound states and energies of the states from continuous spectra above them. The $\epsilon \neq 0$ transforms spectra of Dirac's equation even more, namely appropriate choice gives possibility to make any energy level the lowest one. This possibility was tested and gave positive results. The most important thing is that eigen functions and values (energies) could be found separately from each other as the lowest eigen values of the squared Hamiltonian (4).

6. Conclusions and future perspective

The results of the present work are following. Another way to get spectra and corresponding eigen functions of one electron Dirac's equation is presented. It's shown the absence of spurious states. It was pointed the very attractive method to get highly excited states of the Hamiltonian separately each other as the lowest eigen values of some squared Hamiltonians. The further purpose of author is a generalization of the method for many electron case.

References

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